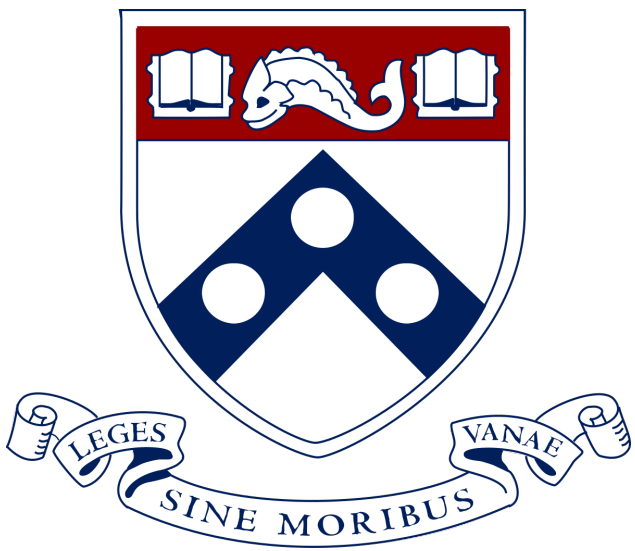
Mathmatial Foundations of Reinforcement Learning

Model-free RL: Q-learning



Yuting Wei

Statistics & Data Science, Wharton
University of Pennsylvania

Fall 2023

Outline

Synchronous Q-learning

Asynchronous Q-learning

Bellman's optimality principle

Bellman operator

$$\mathcal{T}(Q)(s,a) := \underbrace{\mathbb{E}[r(s,a)]}_{\text{immediate reward}} + \gamma \mathop{\mathbb{E}}_{s' \sim P(\cdot|s,a)} \underbrace{\left[\max_{a' \in \mathcal{A}} Q(s',a')\right]}_{\text{next state's value}}$$

- one-step look-ahead

Bellman's optimality equation: $Q^\star$ is the *unique* fixed point to

$$\mathcal{T}(Q^\star) = Q^\star.$$

γ-contraction:

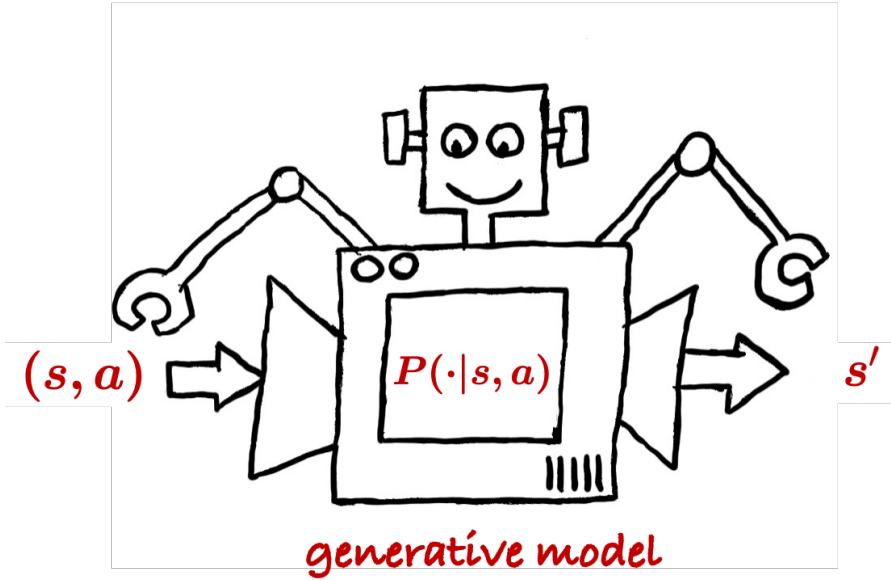
$$\|\mathcal{T}(Q) - \mathcal{T}(Q')\|_\infty \leq \gamma \|Q - Q'\|_\infty$$

Richard Bellman

Synchronous Q-learning

Synchronous sampling with a generative model

— [Kearns and Singh, 1999]



For each state-action pair (s, a), at each time t collect

$$(s, a, s')$$

Question: How many samples are necessary and sufficient to learn the optimal policy without worrying about exploration?

Q-learning: a classical model-free algorithm

Chris Watkins

Peter Dayan

Stochastic approximation for solving the **Bellman equation**

Robbins & Monro, 1951

$$Q = \mathcal{T}(Q)$$

where

$$\mathcal{T}(Q)(s,a) := \underbrace{r(s,a)}_{\text{immediate reward}} + \gamma \mathop{\mathbb{E}}_{s' \sim P(\cdot|s,a)} \underbrace{\left[\max_{a' \in \mathcal{A}} Q(s',a')\right]}_{\text{next state's value}}.$$

Q-learning: a classical model-free algorithm

Chris Watkins

Peter Dayan

Q-learning [Watkins and Dayan, 1992] proceeds as

$$Q_{t+1}(s,a) = \underbrace{(1-\eta_t)Q_t(s,a) + \eta_t \mathcal{T}_t(Q_t)(s,a)}_{\text{draw the transition } (s,a,s') \text{ for all } (s,a)}, \quad t \geq 0$$

$$= Q_t(s,a) + \eta_t \left(r(s,a) + \gamma \max_{a'} Q_t(s',a') - Q_t(s,a) \right)$$

$$\mathcal{T}_t(Q)(s,a) = r(s,a) + \gamma \max_{a'} Q(s',a')$$

$$\mathcal{T}(Q)(s,a) = r(s,a) + \gamma \mathop{\mathbb{E}}_{s' \sim P(\cdot|s,a)} \left[\max_{a'} Q(s',a') \right]$$

Asymptotic convergence

Theorem 1 ([Watkins and Dayan, 1992])

Q-learning converges to the optimal Q-function $Q^\star$ asymptotically with probability 1 as long as

$$\sum_{t=1}^{\infty} \eta_t = \infty, \qquad \sum_{t=1}^{\infty} \eta_t^2 < \infty.$$

- The first condition asks the learning rates to be not too small, while the second condition ensures that they are not too large.
- Many choices of learning rates satisfy this assumption.

What about the finite-time convergence rate of Q-learning?

Prior art: achievability

Question: How many samples are needed for $\|\widehat{Q} - Q^\star\|_\infty \leq \varepsilon$?

paper	learning rates	sample complexity
Even-Dar & Mansour '03	linear: $\frac{1}{t}$	$2^{\frac{1}{1-\gamma}} \frac{\lvert\mathcal{S}\rvert\lvert\mathcal{A}\rvert}{(1-\gamma)^4\varepsilon^2}$
Beck & Srikant '12	constant: $\frac{(1-\gamma)^4\varepsilon^2}{\lvert\mathcal{S}\rvert\lvert\mathcal{A}\rvert}$	$\frac{\lvert\mathcal{S}\rvert^2\lvert\mathcal{A}\rvert^2}{(1-\gamma)^5\varepsilon^2}$
Wainwright '19	rescaled linear: $\frac{1}{1+(1-\gamma)t}$	$\frac{\lvert\mathcal{S}\rvert\lvert\mathcal{A}\rvert}{(1-\gamma)^5\varepsilon^2}$
Chen et al. '20	rescaled linear: $\frac{1}{\frac{1}{(1-\gamma)^2}+(1-\gamma)t}$	$\frac{\lvert\mathcal{S}\rvert\lvert\mathcal{A}\rvert}{(1-\gamma)^5\varepsilon^2}$
Chen et al. '20	constant: $(1-\gamma)^4\varepsilon^2$	$\frac{\lvert\mathcal{S}\rvert\lvert\mathcal{A}\rvert}{(1-\gamma)^5\varepsilon^2}$

A note on the learning rates

Observation: the learning rate schedule $\eta_t = \frac{1}{t}$ leads to a sample complexity that scales exponentially in $\frac{1}{1-\gamma}$.

- Consider the following MDP with a single state $s = 1$, a single action $a = 1$, and $r(1,1) = 1, P(1|1,1) = 1$. Hence,

$$Q^\star(1,1) = \frac{1}{1-\gamma}.$$

- The update rule of Q-learning with learning rate $\eta_t = \frac{1}{t}$ gives

$$\begin{aligned} Q_t(1,1) &= \left(1 - \frac{1}{t}\right) Q_{t-1}(1,1) + \frac{1}{t}\left(1 + \gamma Q_{t-1}(1,1)\right) \\ &= \left(1 - \frac{1-\gamma}{t}\right) Q_{t-1}(1,1) + \frac{1}{t}, \end{aligned}$$

A note on the learning rates - continued

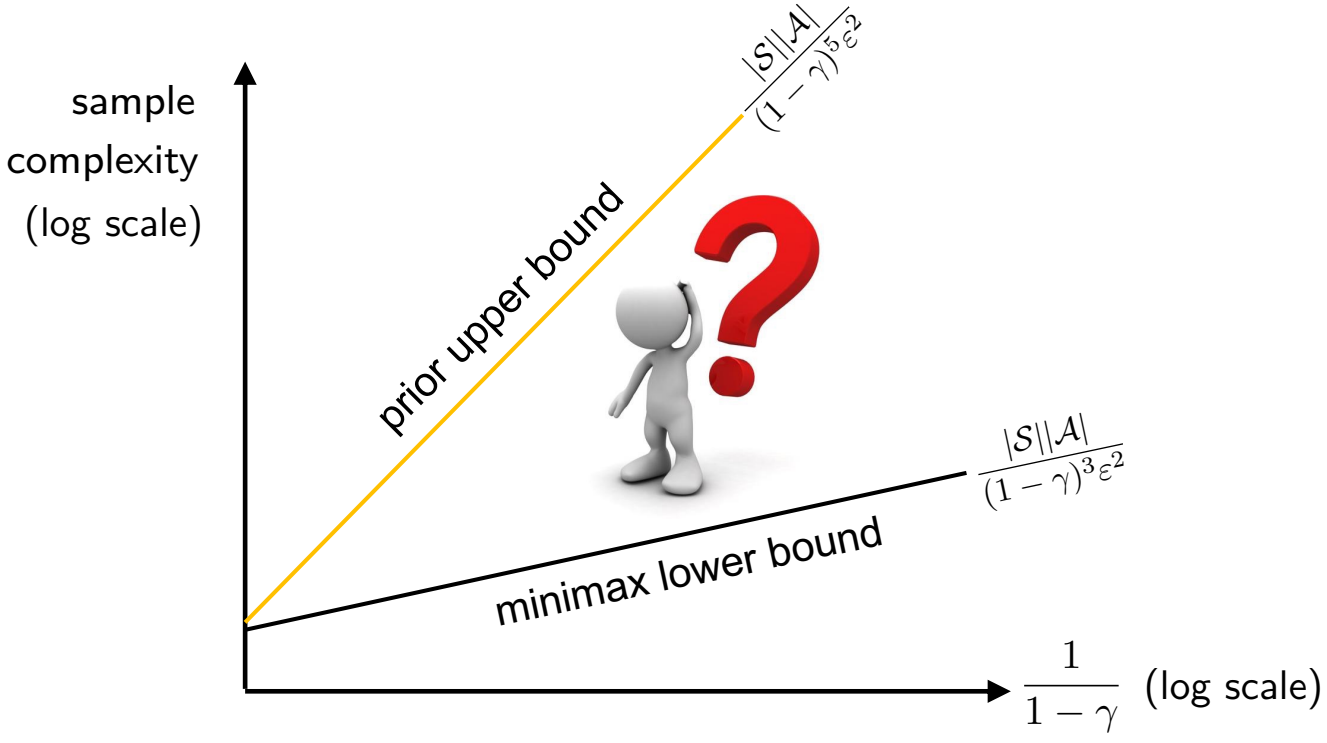
- From simple recursive relations, one can easily check that: when $\gamma \to 1$ and t is not too large, one has

$$\begin{aligned} Q_t - Q^\star &= \prod_{i=1}^{t} \left[1 - \frac{1-\gamma}{i}\right] \cdot [Q_0 - Q^\star] \\ &\approx \left[1 - \sum_{i=1}^{t} \frac{1-\gamma}{i}\right] \cdot [Q_0 - Q^\star] \\ &\approx [1 - (1-\gamma)\log t] \cdot [Q_0 - Q^\star]. \end{aligned}$$

  This essentially implies that one needs to have $t \gtrsim 2^{O(\frac{1}{1-\gamma})}$ iterations to achieve $|Q_t - Q^\star| < \frac{1}{2}|Q_0 - Q^\star|$.

Consequently, the rescaled linear learning rates or constant learning rates provide better alternatives.

Can we close the gap?



All prior results require sample size of at least $\frac{|\mathcal{S}||\mathcal{A}|}{(1-\gamma)^5\varepsilon^2}$!

Is Q-learning sub-optimal, or is it an analysis artifact?

A sharpened sample complexity of Q-learning

Theorem 2 ([Li et al., 2021])

For any $0 < \varepsilon \leq 1$, *Q-learning yields*

$$\|\widehat{Q} - Q^\star\|_\infty \leq \varepsilon$$

with sample complexity at most

$$\widetilde{O}\left(\frac{|\mathcal{S}||\mathcal{A}|}{(1-\gamma)^4\varepsilon^2}\right).$$

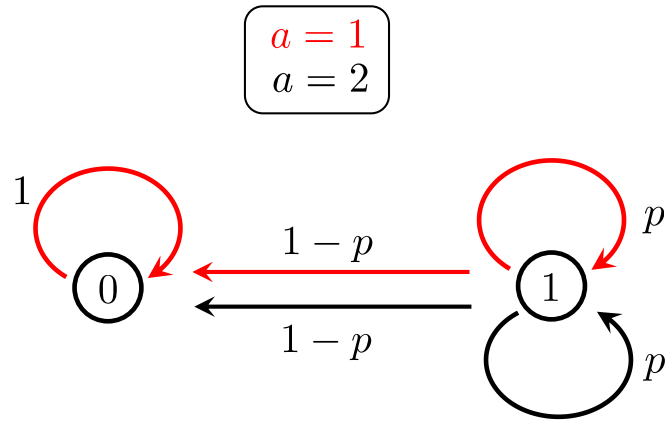
- Improves dependency on effective horizon $\frac{1}{1-\gamma}$
- Allows both constant and rescaled linear learning rate:

$$\frac{1}{1+\frac{c_1(1-\gamma)T}{\log^2 T}} \leq \eta_t \leq \frac{1}{1+\frac{c_2(1-\gamma)t}{\log^2 T}}$$

A curious numerical example

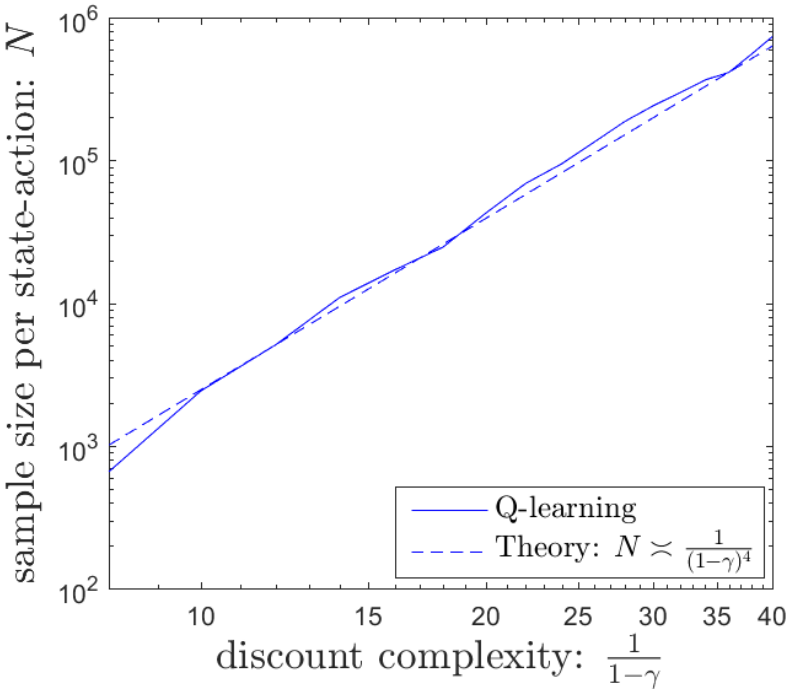
Numerical evidence: $\frac{|\mathcal{S}||\mathcal{A}|}{(1-\gamma)^4\varepsilon^2}$ samples seem necessary . . .

— observed in [Wainwright, 2019a]



$$p = \frac{4\gamma - 1}{3\gamma}$$

$$r(0,1) = 0, \quad r(1,1) = r(1,2) = 1$$



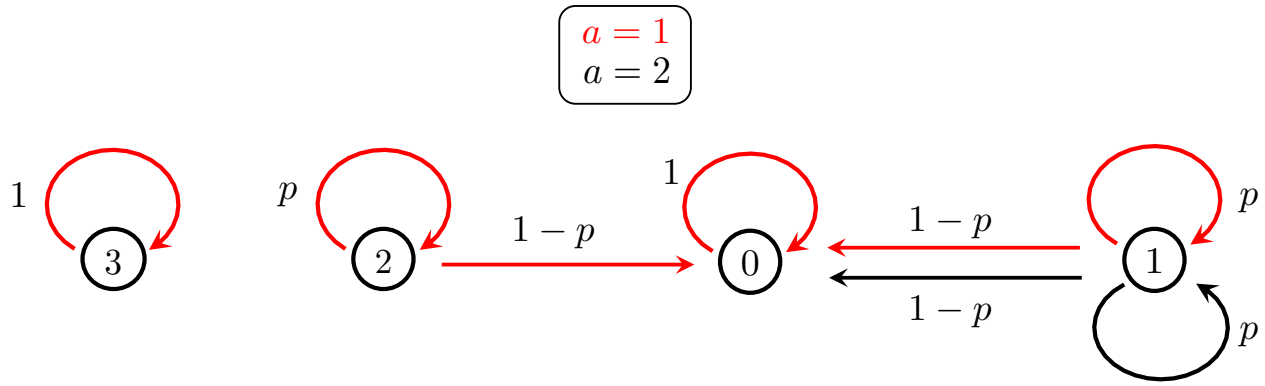
Q-learning is not minimax optimal

Theorem 3 ([Li et al., 2021])

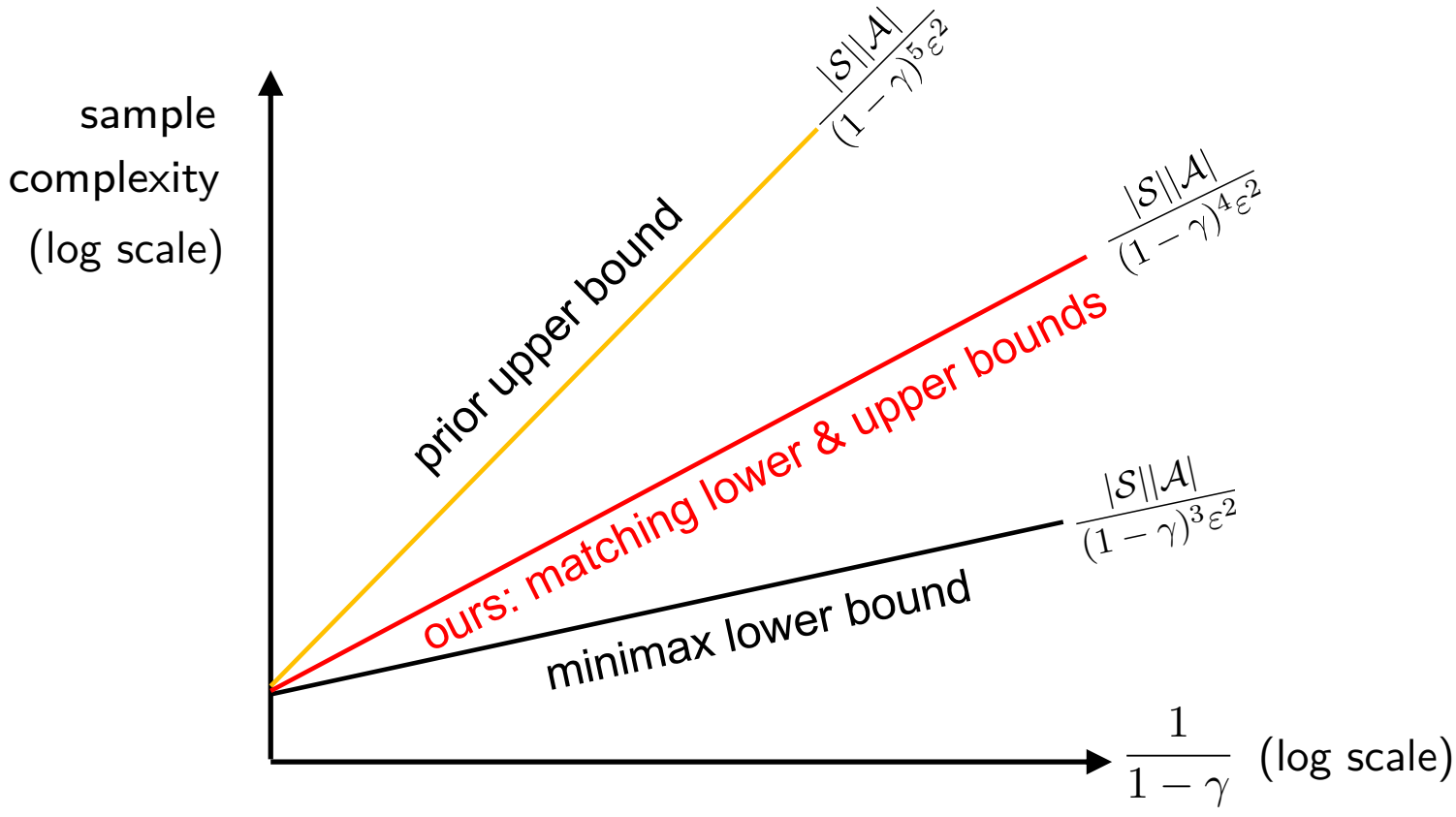
For any $0 < \varepsilon \leq 1$, there exist an MDP such that to achieve $\|\widehat{Q} - Q^\star\|_\infty \leq \varepsilon$, Q-learning needs at least a sample complexity of

$$\widetilde{\Omega}\left(\frac{|\mathcal{S}||\mathcal{A}|}{(1-\gamma)^4\varepsilon^2}\right).$$

- Tight **algorithm-dependent** lower bound
- Holds for both constant and rescaled linear learning rates



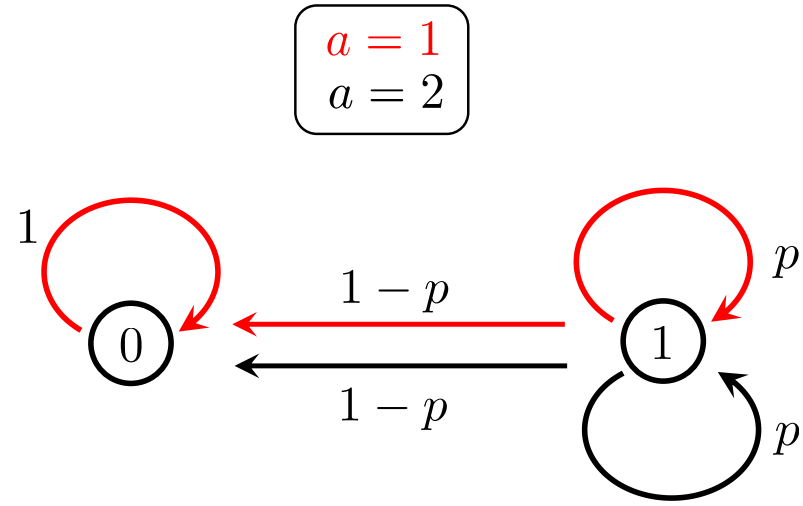
Where we stand now



Q-learning requires a sample size of $\frac{|\mathcal{S}||\mathcal{A}|}{(1-\gamma)^4\varepsilon^2}$.

Why is Q-learning sub-optimal?

Over-estimation of Q-functions [Thrun and Schwartz, 1993, Hasselt, 2010]:



- $\max_{a \in \mathcal{A}} \mathbb{E}X(a)$ tends to be over-estimated (high positive bias) when $\mathbb{E}X(a)$ is replaced by its empirical estimates using a small sample size.

Why is Q-learning sub-optimal?

The over-estimation of Q-functions often gets **worse** with a large number of actions [Van Hasselt et al., 2016].

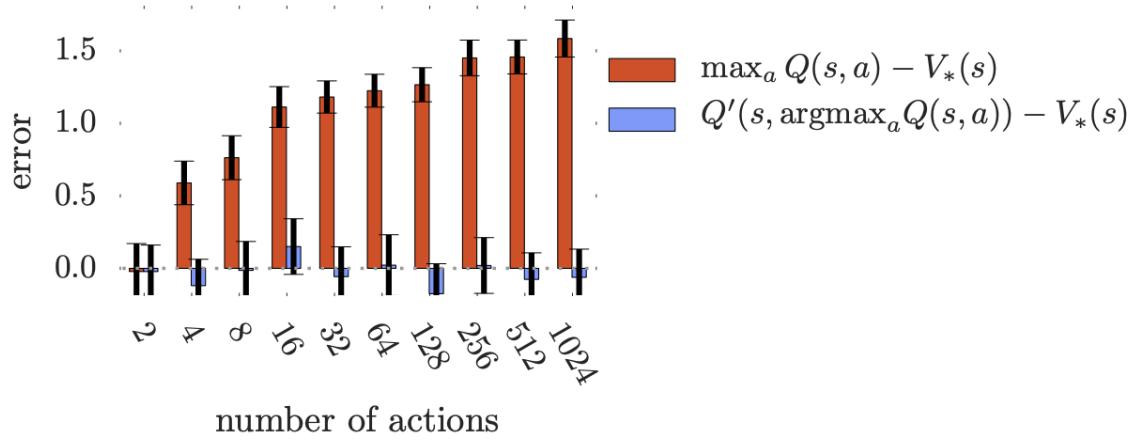


Figure 1: The orange bars show the bias in a single Q-learning update when the action values are $Q(s,a) = V_*(s) + \epsilon_a$ and the errors $\{\epsilon_a\}_{a=1}^m$ are independent standard normal random variables. The second set of action values Q', used for the blue bars, was generated identically and independently. All bars are the average of 100 repetitions.

Double Q-learning

To mitigate the impact of over-estimation, [Hasselt, 2010] proposed **double Q-learning**, which uses two Q-estimates and updates one of them randomly at each round:

$$Q^1(s,a) = (1-\eta_t)Q^1(s,a) + \eta_t \left(r(s,a) + \gamma \max_{a \in \mathcal{A}} Q^2(s',a) \right),$$

or

$$Q^2(s,a) = (1-\eta_t)Q^2(s,a) + \eta_t \left(r(s,a) + \gamma \max_{a \in \mathcal{A}} Q^1(s',a) \right).$$

- Decouple the randomness in value updates and action selection.
- Empirically very successful when integrated with deep RL [Van Hasselt et al., 2016].

TD-learning: when the action space is a singleton

Richard Sutton

Stochastic approximation for solving Bellman equation $V = \mathcal{T}(V)$

$$V_{t+1}(s) = (1-\eta_t)V_t(s) + \eta_t \mathcal{T}_t(V_t)(s)$$
$$= V_t(s) + \eta_t \underbrace{\Big[r(s) + \gamma V_t(s') - V_t(s)\Big]}_{\text{temporal difference}}, \quad t \geq 0$$

$$\mathcal{T}_t(V)(s) = r(s) + \gamma V(s')$$
$$\mathcal{T}(V)(s) = r(s) + \gamma \mathop{\mathbb{E}}_{s' \sim P(\cdot|s)} V(s')$$

Sample complexity of TD-learning

Theorem 4 ([Li et al., 2021])

For any $0 < \varepsilon \leq 1$, *TD-learning yields*

$$\|\widehat{V} - V^\star\|_\infty \leq \varepsilon$$

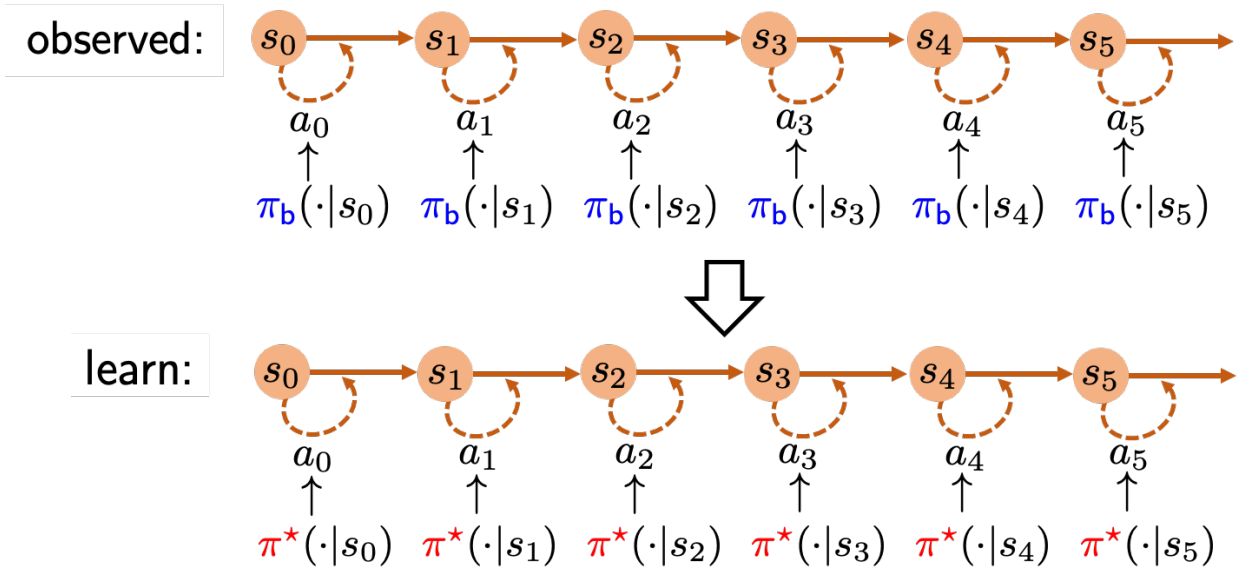
with sample complexity at most

$$\widetilde{O}\left(\frac{|\mathcal{S}|}{(1-\gamma)^3\varepsilon^2}\right).$$

- Near minimax-optimal (matches the minimax lower bound when the action space is a singleton) without the need of averaging or variance reduction.
- Allows both constant and rescaled linear learning rate.

Asynchronous Q-learning

Markovian samples and behavior policy

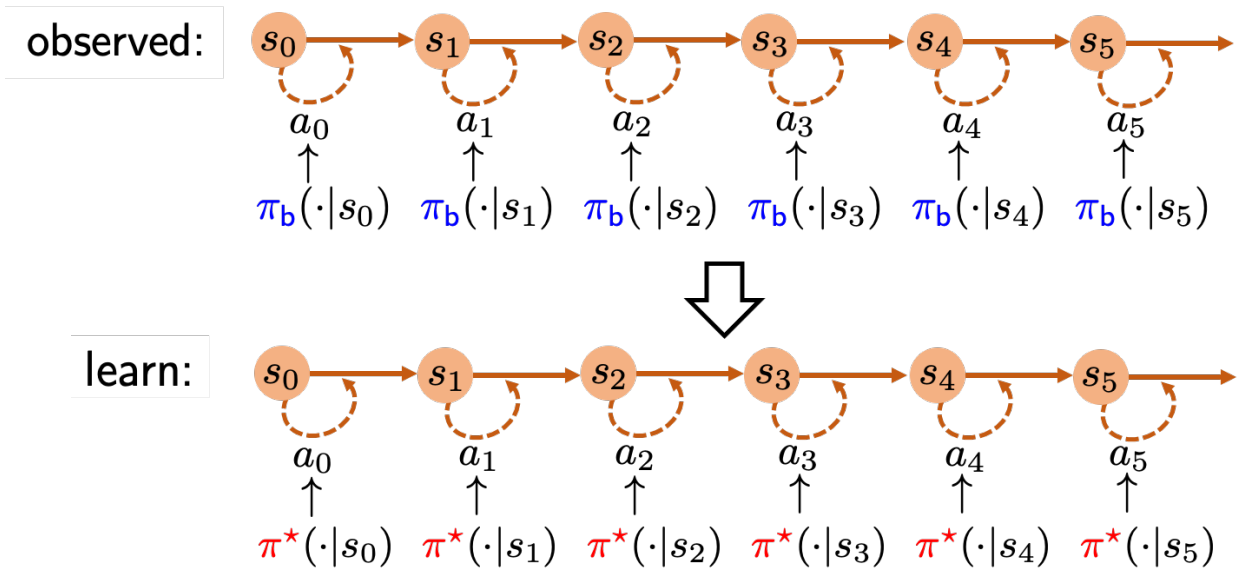


Observed: $\underbrace{\{s_t, a_t, r_t\}_{t\geq 0}}$ generated by behavior policy π_b

stationary Markovian trajectory

Goal: learn optimal value $V^\star$ and $Q^\star$ based on sample trajectory

Key quantities of sample trajectory



- minimum state-action occupancy probability (uniform coverage)

$$\mu_{\mathsf{min}} := \min \underbrace{\mu_{\pi_b}(s,a)}_{\text{stationary distribution}}$$

- mixing time: t_{mix}, which captures the time to reach the steady state

Asynchronous Q-learning

Chris Watkins

Peter Dayan

Stochastic approximation for solving Bellman equation $Q = \mathcal{T}(Q)$

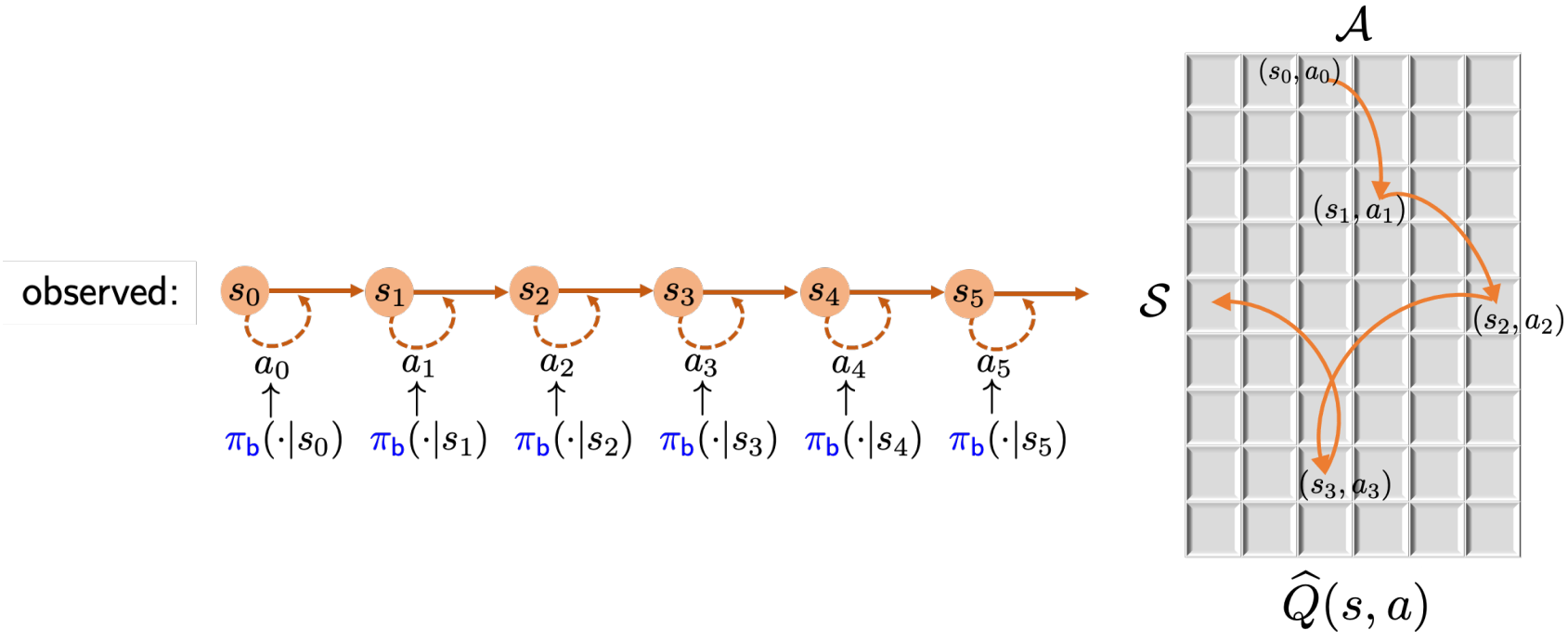
$$\underbrace{Q_{t+1}(s_t, a_t) = (1 - \eta_t) Q_t(s_t, a_t) + \eta_t \mathcal{T}_t(Q_t)(s_t, a_t)}, \quad t \geq 0$$

only update (s_t, a_t)-th entry

$$\mathcal{T}_t(Q)(s_t, a_t) = r(s_t, a_t) + \gamma \max_{a'} Q(s_{t+1}, a')$$

$$\mathcal{T}(Q)(s, a) = r(s, a) + \gamma \mathop{\mathbb{E}}_{s' \sim P(\cdot|s,a)} \Big[\max_{a'} Q(s', a') \Big]$$

Q-learning on Markovian samples



- **asynchronous:** only a single entry is updated each iteration
  - resembles Markov-chain *coordinate descent*
- **off-policy:** target policy $\pi^\star \neq$ behavior policy π_b

Sample complexity of asynchronous Q-learning

Theorem 5 ([Li et al., 2022])

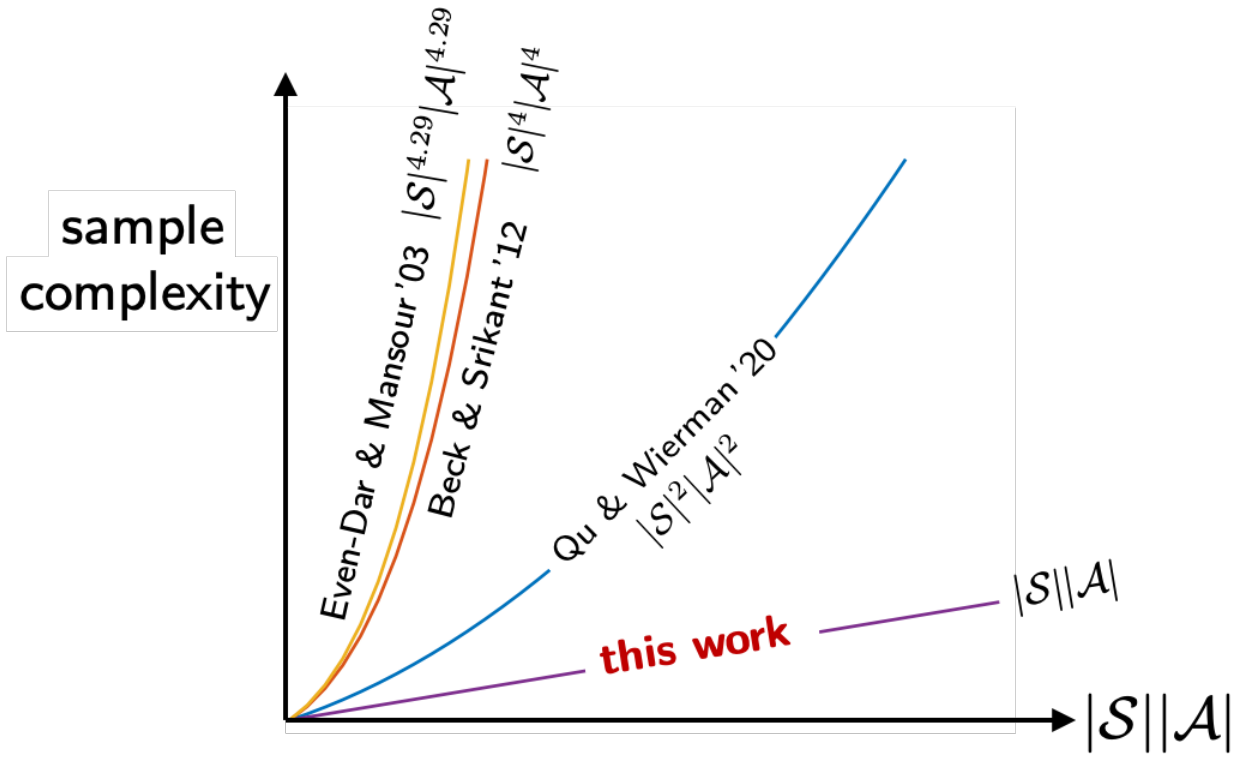
For any $0 < \varepsilon \leq \frac{1}{1-\gamma}$, *sample complexity of async Q-learning to yield* $\|\widehat{Q} - Q^\star\|_\infty \leq \varepsilon$ *is at most (up to some log factor)*

$$\frac{1}{\mu_{\mathsf{min}}(1-\gamma)^5\varepsilon^2} + \frac{t_{\mathsf{mix}}}{\mu_{\mathsf{min}}(1-\gamma)}$$

- The first term can be improved further to $\frac{1}{\mu_{\mathsf{min}}(1-\gamma)^4\varepsilon^2}$ [Li et al., 2021] for $0 < \varepsilon \leq 1$.
- Prior art $\frac{t_{\mathsf{mix}}}{\mu_{\mathsf{min}}^2(1-\gamma)^5\epsilon^2}$ (Qu and Wierman'20)

A collection of prior art: async Q-learning

Question: how many samples are needed to ensure $\|\widehat{Q} - Q^\star\|_\infty \leq \varepsilon$?

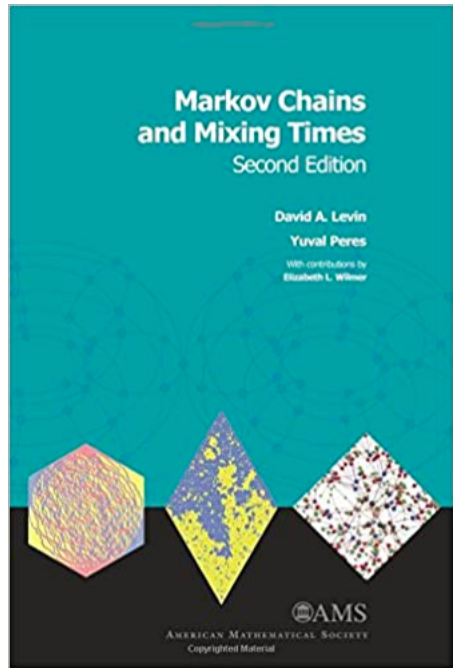


if we take $\mu_{\min} \asymp \frac{1}{|\mathcal{S}||\mathcal{A}|}$, $t_{\text{cover}} \asymp \frac{t_{\text{mix}}}{\mu_{\min}}$

All prior results require sample size of at least $t_{\text{mix}}|\mathcal{S}|^2|\mathcal{A}|^2$!

Effect of mixing time on sample complexity

$$\frac{1}{\mu_{\mathsf{min}}(1-\gamma)^5\varepsilon^2} + \frac{t_{\mathsf{mix}}}{\mu_{\mathsf{min}}(1-\gamma)}$$



- reflects cost taken to reach steady state
- one-time expense (almost independent of ε)
  — it becomes amortized as algorithm runs

Minimax lower bound

minimax lower bound
(Azar et al. '13)

$$\frac{1}{\mu_{\min}(1-\gamma)^3\varepsilon^2}$$

asyn Q-learning
(ignoring dependency on t_{mix})

$$\frac{1}{\mu_{\min}(1-\gamma)^5\varepsilon^2}$$

Can we improve dependency on **discount complexity** $\frac{1}{1-\gamma}$?

One strategy: variance reduction

—[Wainwright, 2019b, Li et al., 2022]

Variance-reduced Q-learning updates

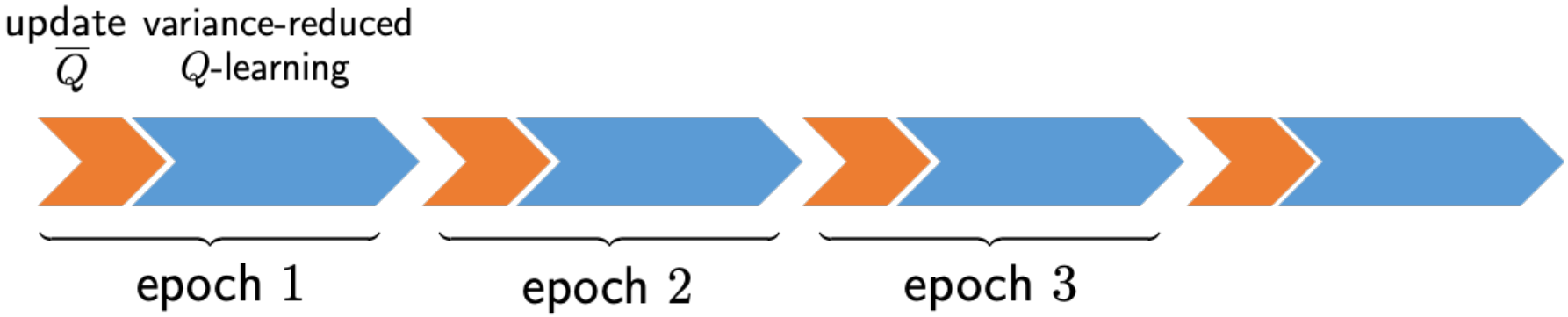
$$Q_t(s_t,a_t) = (1-\eta)Q_{t-1}(s_t,a_t) + \eta\Big(\mathcal{T}_t(Q_{t-1}) \underbrace{-\mathcal{T}_t(\overline{Q}) + \widetilde{\mathcal{T}}(\overline{Q})}_{\text{use } \overline{Q} \text{ to help reduce variability}}\Big)(s_t,a_t)$$

- $\overline{Q}$: some reference Q-estimate
- $\widetilde{\mathcal{T}}$: empirical Bellman operator (using a batch of samples)

— inspired by Johnson and Zhang'13

Variance-reduced Q-learning

—[Wainwright, 2019b, Li et al., 2022]



for each epoch

1. update $\overline{Q}$ and $\widetilde{T}(\overline{Q})$
2. run variance-reduced Q-learning updates

Main result: ℓ_∞-based sample complexity

Theorem 6 ([Li et al., 2022])

For any $0 < \varepsilon \leq 1$, sample complexity for ***(async) variance-reduced Q-learning*** *to yield $\|\widehat{Q} - Q^\star\|_\infty \leq \varepsilon$ is at most on the order of*

$$\frac{1}{\mu_{\mathsf{min}}(1-\gamma)^3\varepsilon^2} + \frac{t_{\mathsf{mix}}}{\mu_{\mathsf{min}}(1-\gamma)}$$

- more aggressive learning rates: $\eta_t \equiv \min\left\{\frac{\cancel{(1-\gamma)^4}(1-\gamma)^2}{\gamma^2}, \frac{1}{t_{\mathsf{mix}}}\right\}$
- minimax-optimal for $0 < \varepsilon \leq 1$

References I

Hasselt, H. (2010).
Double Q-learning.
Advances in neural information processing systems, 23:2613–2621.

Kearns, M. J. and Singh, S. P. (1999).
Finite-sample convergence rates for Q-learning and indirect algorithms.
In *Advances in neural information processing systems*, pages 996–1002.

Li, G., Cai, C., Chen, Y., Wei, Y., and Chi, Y. (2021).
Is Q-learning minimax optimal? a tight sample complexity analysis.
arXiv preprint arXiv:2102.06548.

Li, G., Wei, Y., Chi, Y., Gu, Y., and Chen, Y. (2022).
Sample complexity of asynchronous Q-learning: Sharper analysis and variance reduction.
IEEE Transactions on Information Theory, 68(1):448–473.

Thrun, S. and Schwartz, A. (1993).
Issues in using function approximation for reinforcement learning.
In *Proceedings of the Fourth Connectionist Models Summer School*, volume 255, page 263.
Hillsdale, NJ.

Van Hasselt, H., Guez, A., and Silver, D. (2016).
Deep reinforcement learning with double Q-learning.
In *Proceedings of the AAAI conference on artificial intelligence*, volume 30.

References II

Wainwright, M. J. (2019a).
Stochastic approximation with cone-contractive operators: Sharp ℓ_∞-bounds for Q-learning.
arXiv preprint arXiv:1905.06265.

Wainwright, M. J. (2019b).
Variance-reduced Q-learning is minimax optimal.
arXiv preprint arXiv:1906.04697.

Watkins, C. J. and Dayan, P. (1992).
Q-learning.
Machine learning, 8(3-4):279–292.